

Nonlinear regression

Stat 94
11-21-17

①

Consider the model $y = \beta e^{\alpha x} + \varepsilon$

$$SSE = \sum_{i=1}^n (y_i - \beta e^{\alpha x_i})^2$$

$$\frac{\partial SSE}{\partial \beta} = \sum_{i=1}^n 2(y_i - \beta e^{\alpha x_i}) e^{\alpha x_i} \stackrel{\text{set}}{=} 0$$

$$\sum_{i=1}^n y_i e^{\alpha x_i} = \beta \sum_{i=1}^n e^{2\alpha x_i}$$

$$\hat{\beta} = \frac{\sum_{i=1}^n y_i e^{\hat{\alpha} x_i}}{\sum_{i=1}^n e^{2\hat{\alpha} x_i}}$$

$$\frac{\partial SSE}{\partial \alpha} = \sum_{i=1}^n 2(y_i - \beta e^{\alpha x_i})(+\beta e^{\alpha x_i} x_i) \stackrel{\text{set}}{=} 0 \quad (2)$$

$$\beta \sum_{i=1}^n y_i x_i e^{\alpha x_i} - \beta^2 \sum_{i=1}^n x_i e^{2\alpha x_i} = 0$$

If $\beta \neq 0$, divide both sides by β

$$\sum_{i=1}^n y_i x_i e^{\alpha x_i} - \beta \sum_{i=1}^n x_i e^{2\alpha x_i} = 0$$

$\hat{\alpha}$ solve for α numerically

Ridge regression

③

Recall $\hat{\beta} = (X'X)^{-1} X'Y$

Consider $\hat{\beta}_R = (X'X + \underset{\substack{\uparrow \\ \text{constant}}}{kI})^{-1} X'Y$

let $MSE(\hat{\beta}) = E[\hat{\beta} - \beta]^2$

"mean squared error"

$$MSE(\hat{\beta}) = E[\underbrace{\hat{\beta} - E(\hat{\beta})}_{\text{error}} + \underbrace{E(\hat{\beta}) - \beta}_{\text{bias}}]^2 \quad \textcircled{4}$$

$$= E[\hat{\beta} - E(\hat{\beta})]^2 + E[E(\hat{\beta}) - \beta]^2 \\ + 2 E[(\hat{\beta} - E(\hat{\beta})) (E(\hat{\beta}) - \beta)]$$

$$= V[\hat{\beta}] + \text{Bias}^2(\hat{\beta}) + 2(E(\hat{\beta}) - \beta) \underbrace{E[\hat{\beta} - E(\hat{\beta})]}_0$$

$$\therefore MSE(\hat{\beta}) = V[\hat{\beta}] + \text{Bias}^2(\hat{\beta})$$

So, our goal is to find k in ridge regression that will minimize $MSE(\hat{\beta}_R)$

Proposed in 1970 by Hoerl & Kennard

$$\begin{aligned} E[\hat{\beta}_R] &= E[(X'X + kI)^{-1}X'Y] \\ &= (X'X + kI)^{-1}X' E[Y] \\ &= (X'X + kI)^{-1}X' E[X\beta + \varepsilon] \\ &= (X'X + kI)^{-1}X'X\beta \end{aligned}$$

$$\begin{aligned} \text{Bias}(\hat{\beta}_R) &= E[\hat{\beta}_R] - \beta \\ &= [(X'X + kI)^{-1}X'X - I]\beta \\ &= (X'X + kI)^{-1}[X'X - (X'X + kI)]\beta \\ &= -k(X'X + kI)^{-1}\beta \end{aligned}$$

$$\begin{aligned} V[\hat{\beta}_R] &= V[(X'X + kI)^{-1}X'Y] \\ &= V[(X'X + kI)^{-1}(X'X)(\underbrace{(X'X)^{-1}X'Y}_{\hat{\beta}})] \end{aligned}$$

$$= (X'X + kI)^{-1} X'X \underbrace{\text{Cov}(\hat{\beta})}_{\sigma^2(X'X)^{-1}} X'X (X'X + kI)^{-1} \quad (7)$$

$$= \sigma^2 (X'X + kI)^{-1} X'X (X'X + kI)^{-1}$$

Hoerl & Kennard proposed minimizing the trace of

$$V[\hat{\beta}_R] + [\text{Bias}(\hat{\beta}_R)]' \text{Bias}(\hat{\beta}_R)$$

They proved (1) There exists a value of k such that $\text{MSE}(\hat{\beta}_R) < V[\hat{\beta}]$

(2) As $k \uparrow$, $R^2 \downarrow$

(8)

Logistic regression

$$Y = X\beta + \varepsilon$$

What if Y only takes on the values 0 and 1?

$V(Y) = V(\varepsilon)$, so ε has a Bernoulli distribution, where p is the prob that $Y=1$

But p depends on X , so $V(\varepsilon)$ is not constant

What if we try to predict $p = P(Y=1)$
instead of predicting Y ?

⑨

$p = X\beta + \varepsilon$ We may still get
predicted values > 1 or < 0

Try $\ln\left(\frac{p}{1-p}\right) = X\beta + \varepsilon$

logit(p)

This is called the logistic
regression model

i.e., you are predicting the natural log of the odds
of success

⑩

$$\text{logit}(p) = w$$

$$\ln\left(\frac{p}{1-p}\right) = w \quad \frac{p}{1-p} = e^w$$

$$p = e^w - pe^w$$

$$p(1 + e^w) = e^w$$

$$p = \frac{e^w}{1 + e^w}$$

$$\text{So } \hat{p} = \frac{e^{X\hat{\beta}}}{1 + e^{X\hat{\beta}}}$$

How is $\hat{\beta}$ found?

(11)

Y has a Bernoulli distribution,

$$\text{so } P(Y=y) = p^y (1-p)^{1-y}$$

The likelihood function is the product of these probabilities

$$L = \prod_{i=1}^n p_i^{y_i} (1-p_i)^{1-y_i}$$

where $p_i = \frac{e^{x_i \beta}}{1 + e^{x_i \beta}}$

Then, using numerical methods, find the $\hat{\beta}$ which maximizes L .

(12)

- 6.1** Perform a thorough influence analysis of the solar thermal energy test data given in Table B.2. Discuss your results.

Note: check my webpage for a link to the Excel file called TableB2.xlsx.

- 7.6** The carbonation level of a soft drink beverage is affected by the temperature of the product and the filler operating pressure. Twelve observations were obtained and the resulting data are shown below.

Carbonation, y	Temperature, x_1	Pressure, x_2
2.60	31.0	21.0
2.40	31.0	21.0
17.32	31.5	24.0
15.60	31.5	24.0
16.12	31.5	24.0
5.36	30.5	22.0
6.19	31.5	22.0
10.17	30.5	23.0
2.62	31.0	21.5
2.98	30.5	21.5
6.92	31.0	22.5
7.06	30.5	22.5

- Fit a second-order polynomial.
- Test for significance of regression.
- Test for lack of fit and draw conclusions.
- Does the interaction term contribute significantly to the model?
- Do the second-order terms contribute significantly to the model?